

Diethyl butanedioate  
123-25-1 | DTXSID2038732

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.04

Global applicability domain: Inside

Local applicability domain index: 7.10e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethyl butanedioate</div> <div>Measured: 1.20</div> <div>Predicted: 1.04</div>	<div>Image not found</div> <div>Dimethyl adipate</div> <div>Measured: 1.03</div> <div>Predicted: 1.03</div>	<div>Image not found</div> <div>Diethyl propanedioate</div> <div>Measured: 0.96</div> <div>Predicted: 8.73e-01</div>
<div>Image not found</div> <div>Dimethyl glutarate</div> <div>Measured: 0.62</div> <div>Predicted: 7.46e-01</div>	<div>Image not found</div> <div>Methyl 6-oxoheptanoate</div> <div>Measured: 0.55</div> <div>Predicted: 8.61e-01</div>	